

KFKI-1981-72

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Hungarian Academy of Sciences

CENTRAL
RESEARCH
INSTITUTE FOR
PHYSICS

BUDAPEST

2017

KFKI-1981-72

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To appear in the Zeitschrift für Physik B

HU ISSN 0368 5330
ISBN 963 371 854 6

On leave of absence from the Central Research Institute for Physics, Budapest

ABSTRACT

Earlier studies of the triangular lattice antiferromagnet and the fully frustrated model on the square lattice proved that in these models the pair correlation $\langle S_0 S_r \rangle$ decreases asymptotically as $r^{-1/2}$ at zero temperature. In the present paper the existence of two and higher dimensional models is shown in which the frustration is so strong that it destroys the phase transition even at $T=0$: the correlation length remains finite. The influence of this "superfrustration" on the free energy and on the ground state properties is also discussed.

АННОТАЦИЯ

Исследования корреляционной функции $\langle S_0 S_r \rangle$ в треугольной антиферромагнитной и полностью фрустрационной, квадратной решетке показали, что она асимптотически пропорциональна $r^{-1/2}$ при нулевой температуре. В настоящей статье показано, что при размерности пространства два и больше существуют такие сильно фрустрационные модели, в которых нет фазового перехода даже при нулевой температуре; корреляционный радиус остается конечным. Эффект "суперфрустрации" проявляется и в свободной энергии и свойствах основного состояния.

KIVONAT

Korábbi vizsgálatok, melyeket a háromszögrács-antiferromágnesen, valamint a négyzetrács fölötti teljesen frusztrált modellen végeztek, azt bizonyítják, hogy az $\langle S_0 S_r \rangle$ párkorreláció aszimptotikusan arányos $r^{-1/2}$ -del nulla hőmérsékleten. Az alábbiakban megmutatom, hogy két és bármely nagyobb dimenzióban léteznek olyan erősen frusztrált modellek, melyekben $T=0$ -n sincs fázisátmenet: a korrelációs hossz véges marad. Ez a "szuperfrusztráció" nyomot hagy a szabadenergián és az alapállapot tulajdonságokon is.

1. Introduction

Ising models with competing interactions have attracted a considerable interest since the possible relevance of frustration to the properties of spin glasses has been pointed out by Toulouse [1]. Frustration is an extreme manifestation of the competition among the interactions, leading to an accidental (not-symmetry-imposed) degeneracy of the ground state. In the most spectacular cases, this degeneracy results in a macroscopic entropy at zero temperature ($T = 0$) and the disappearance of the phase transitions for $T > 0$: I mention here the antiferromagnetic model on the triangular lattice [2] (denoted by TAF), the antiferromagnetic and fully frustrated models on the Kagomé lattice [3] (KAF and KFF respectively) and the fully frustrated model on the square lattice [4] (SFF). In the case of two dimensional models with periodic nearest neighbour pair interactions, as in the above examples, the free energy can be calculated exactly by Onsager's method and the zero point entropy can be inferred from it. Spins not being frozen-in at $T = 0$, the correlation functions may also be subject to interest. While the absence of a local magnetization and, therefore, the decay of the correlations with increasing distance is rather obvious (though, as I will point out later, the boundary conditions play a non-trivial role), one cannot simply guess the rate of this decay. The free energy of any reasonable statistical ensemble is singular at $T = 0$ - this follows from the essential singularity of $\exp(-H/k_B T)$ - so one would expect a power-law behaviour of the correlations as at a critical temperature. The result of Stephenson [5] for the TAF model supports this expectation: $\langle S_0 S_r \rangle \sim r^{-\eta}$ at $T = 0$, with $\eta = 1/2$. In two recent papers, Southern et al. [6] and Forgacs [7] studied the correlations of the SFF model. In the first paper, the authors found a power-law decay with $\zeta = 1/4$. Forgacs' more careful analysis lead to $\zeta = 1/2$. Considering these results, obtained for fully frustrated models, together with the fact that in the absence of frustration there is a long range order at $T = 0$, one might think that the correlation length

must be infinite in all Ising models at zero temperature.

In the present paper it is shown that in certain models the frustration may be so strong that the correlations decay exponentially at any temperature, including $T = 0$. The term "superfrustration model" will be applied to models of frustration which do not undergo any phase transition and in which the correlation length is finite at $T = 0$. The first examples for such models were given in an earlier paper [8] where a method for discussing the analytical properties of the free energy and the correlations in the case of frustration was developed. The present work generalizes the results of [8] and uses a simplified argument to show that the following conditions are sufficient for the superfrustration:

In the given model there exists a "dominant" subset, S , of plaquettes so that

- (i) S contains triangles and/or squares ;
- (ii) S covers the whole set of bonds disjointly ;
- (iii) S is weakly connected in the sense that
 - a) every lattice site is shared by at most two dominant plaquettes;
 - b) N_n , the number of closed chains formed by a given dominant plaquette and $n-1$ other elements of S , does not increase very rapidly with n ;
- (iv) there are only nearest neighbour pair interactions, J_{ij} , defined so that every plaquette of S is frustrated.

One can formulate (iii/b) more quantitatively:

$$(iii/b) \quad \sum_n N_n \frac{x_S^n}{(1-\epsilon)^{n-1}} < \epsilon < 1$$

can be solved for ϵ . Here

$$x_S = (1/3)^\alpha (1/2)^{1-\alpha}$$

if S is a homogeneous mixture of triangles and squares and the proportion of the former is α . These conditions can be satisfied in two and higher dimensions, therefore, superfrustration exists in any dimension greater

than one. For a two-dimensional example, I mention that (i) - (iii) are fulfilled for the Kagomé lattice if S is chosen to be the whole set of triangles. If, in addition, the interactions are defined so that every triangle is frustrated, the model will be superfrustrated. In particular, this is true for the KFF model and also for the KAF model where the hexagonal plaquettes are non-frustrated. The example of the KFF model shows that the conjecture [7], according to which all two-dimensional fully frustrated models form a universality class characterized by the decay $\langle S_0 S_r \rangle \sim r^{-1/2}$ at $T = 0$, does not hold. It is worth mentioning that the SFF model, which is not superfrustrated, violates (iii/b); this shows the "sharpness" of this condition.

The appearance of a finite correlation length despite of a singularity in the free energy runs against the intuition. These facts will be reconciled by showing that the singularity of the free energy at $T = 0$ is relatively mild, essentially of the same type as that produced by a single Ising spin in an external field.

It should be emphasized that the conditions (i) - (iv) are not necessary to the superfrustration: each of them could be weakened but the formulation of the conditions would become more complicated. An important feature of these conditions is that they provide us with a recipe for constructing superfrustrated models. A non-constructive condition for the superfrustration which is, however, both sufficient and necessary, can also be obtained. At zero temperature, the only configurations available for a system are the ground states of this system. The different behaviour of the correlations at $T = 0$, found in the models mentioned above, must therefore be the consequence of a qualitative difference between the sets of the ground states. I believe that this consists of the fact that the family of the ground states in both the TAF and SFF models is unstable with respect to boundary perturbations whereas that of the KFF, KAF etc. models is stable. The instability means that the ground state degeneracy can be split up by a suitable choice of the boundary condition. In other words, the equilibrium state at $T = 0$ is not unique for the TAF and SFF

models, while it is apparently unique for the KFF and KAF models. The uniqueness of the zero temperature equilibrium state, together with the non-uniqueness of the ground state configurations, seems to be sufficient and necessary for the superfrustration.

The paper is organized as follows. In Section 2 the pair correlations in models on the Kagomé lattice are studied by using vacuum boundary condition and it is shown that $\langle S_0 S_r \rangle$ decays exponentially with increasing r at any $T \geq 0$, if all the triangles are frustrated. The extension of the proof to all models of the type (i) - (iv) is discussed at the end of the section. I omit the proof of the exponential clustering of general n -point correlations; in the case of the Kagomé lattice models, this was done in [8]. Section 3 presents the results on the analyticity properties of the free energy. In Section 4, I discuss the effect of the boundary conditions on the ground state properties and give a qualitative argument predicting a power-law decay of the correlation for the TAF and SFF models and an exponential decay for the KFF, KAF etc. models. Finally, Section 5 contains the summary of the paper.

2. Decay of the Pair Correlations on the Kagomé Lattice

Let us consider the correlations of the spins belonging to the sites i and j .

$$\langle S_i S_j \rangle = \frac{\sum_{\{S\}} S_i S_j \exp(\beta \sum_{\langle kl \rangle} J_{kl} S_k S_l)}{\sum_{\{S\}} \exp(\beta \sum_{\langle kl \rangle} J_{kl} S_k S_l)} \quad (1)$$

Applying the usual transformation

$$\begin{aligned} \exp(\beta J_{kl} S_k S_l) &= \cosh \beta J_{kl} (1 + S_k S_l \tanh \beta J_{kl}) \\ &\equiv \cosh \beta J_{kl} (1 + S_k S_l z_{kl}) \end{aligned} \quad (2)$$

and summing over the spin configurations we obtain

$$\langle S_i S_j \rangle = \frac{\sum_{g \in G_{ij}} \prod_{\langle kl \rangle \in g} z_{kl}}{\sum_{g \in G} \prod_{\langle kl \rangle \in g} z_{kl}} \quad (3)$$

Here G_{ij} and G contain certain graphs built up from the edges of the lattice: the graphs of G are unions of closed loops and those of G_{ij} are formed from closed loops and from a string connecting the sites i and j .

Every edge of the Kagomé lattice belongs to a unique triangle, therefore the set of all edges can be considered as the union of triangles. Let us assume that our system consists of N triangles: B^1, \dots, B^N . The triangle B^α ($\alpha = 1, \dots, N$) is the collection of three bonds $\langle k_\alpha l_\alpha \rangle$, $\langle l_\alpha m_\alpha \rangle$ and $\langle m_\alpha k_\alpha \rangle$. Dividing the numerator and denominator of (3) by

$$\prod_{\alpha=1}^N (1 + z_{k_\alpha l_\alpha} z_{l_\alpha m_\alpha} z_{m_\alpha k_\alpha})$$

and performing some algebra we arrive at

$$\langle S_i S_j \rangle = \frac{\sum'_{g \in G_{ij}} \prod_{\langle kl \rangle \in g} \zeta_{kl}}{\sum'_{g \in G} \prod_{\langle kl \rangle \in g} \zeta_{kl}} \quad (4)$$

Here

$$\zeta_{kl} = \frac{z_{kl} + z_{lm} z_{mk}}{1 + z_{kl} z_{lm} z_{mk}} = \langle S_k S_l \rangle_{B^\alpha} \quad (5)$$

is a correlation function on the triangle B^α containing the bonds $\langle kl \rangle$, $\langle lm \rangle$, and $\langle mk \rangle$ and the prime indicates that the summations are restricted to graphs using at most one edge from any triangle. Our gain is twofold with the introduction of the new variables (5). Firstly, the number of terms in the sums of (4) is less than that in Eq. (3). Secondly, if the triangle B^α is frustrated then for any $\langle kl \rangle \in B^\alpha$ the magnitude of ζ_{kl} varies in the interval $[0, 1/3]$ with β running from 0 to $+\infty$, while $|z_{kl}|$ covers the whole interval $[0, 1]$. Indeed,

$$|\zeta_{kl}| = |(\text{sgn } J_{kl}) \frac{w}{1 + w + w^2}| \leq 1/3 \quad (6)$$

if

$$\text{sgn} (J_{kl} J_{lm} J_{mk}) = -1$$

and

$$\tanh \beta |J_{kl}| = w$$

for any $\langle kl \rangle \in B^\alpha$. One may, therefore, hope for a better convergence of the sums in (4) than of those in (3). Indeed, that is what we find.

The summation in the numerator of (4) goes over all the "two-leg" graphs having their legs in i and j . Each such graph consists of a connected two-leg graph and a number of closed loops. The contribution of these latter cancels a suitable factor of the denominator, thus leaving

$$\langle S_i S_j \rangle = \sum_{n \geq 1} \sum'' \{ \langle k_{\alpha_1} l_{\alpha_1} \rangle, \dots, \langle k_{\alpha_n} l_{\alpha_n} \rangle \} \in G_{ij} \frac{\zeta_{k_{\alpha_1} l_{\alpha_1}}}{1 + t_{-\alpha_1}^{\alpha_1}} \dots \frac{\zeta_{k_{\alpha_n} l_{\alpha_n}}}{1 + t_{-\alpha_1 - \alpha_2 \dots - \alpha_n}^{\alpha_n}} \quad (7)$$

The double prime indicates that one has to sum over the strings connecting i and j and containing at most one edge from any given triangle. Furthermore,

$$t_{-\alpha_1 - \alpha_2 \dots - \alpha_j}^{\alpha_j} = \sum_{\langle kl \rangle \in B^{\alpha_j}} \zeta_{kl} \langle S_k S_l \rangle (B^{\alpha_1} \cup \dots \cup B^{\alpha_j})^c \quad (8)$$

that is, $t_{-\alpha_1 \dots - \alpha_j}^{\alpha_j}$ is the linear combination of three first neighbour correlation functions which do not depend on the interactions belonging to the triangles $B^{\alpha_1}, \dots, B^{\alpha_j}$.

Let us apply (7) to $\{i, j\} = \langle ij \rangle$, i.e., to a bond. Then a first neighbour correlation, depending on the interactions of B^1, \dots, B^N , is expressed in terms of other first neighbour correlations, each depending on the bonds of a number of triangles smaller than N . If (7) is written for the three edges of a triangle and a linear combination

of these equations with the corresponding weights ε_{k1} is taken, then a recursion relation for the functions t (Eq. 8) is obtained. This can be used to give a uniform bound on $|t_{-\alpha_1 \dots -\alpha_j}^{\alpha_j}|$, valid for any set of triangles and for any T . One can see from Eqs. (6), (7) and (8) that this bound is ε if the condition (iii/b) is satisfied for ε . Now $x_S = 1/3$, $N_{2n+1} = 0$ and $N_{2n} < 2^{2n}$ asymptotically. To find a solution for (iii/b), it is necessary to use the much smaller exact values of N_{2n} for several small values of n . One then obtains that $\varepsilon = 0.1$ satisfies (iii/b) and hence

$$|t_{-\alpha_1 \dots -\alpha_j}^{\alpha_j}| \leq 0.1 \quad (9)$$

for any $\alpha_1, \dots, \alpha_j$. To estimate the pair correlations, we still need the bound

$$N_n^{ij} < 2^n \quad (10)$$

where N_n^{ij} is the number of sets of length n occurring in the summation (7). Applying the estimates (6), (9) and (10) in Eq. (7) we get the final result

$$|<S_i S_j>| \leq \sum_{n \geq |i-j|} 2^n \left(\frac{1/3}{1-0.1}\right)^n < 4 \times 0.74^{|i-j|} \quad (11)$$

which is valid for any $T \geq 0$.

Thinking over the properties used to derive (11) one finds indeed those which were enumerated in the Introduction. This shows that the proof can be transferred to any model satisfying (i) - (iv). The substitution of the triangular plaquettes with squares is allowed because the diagonal pair-correlations and the four-point correlation vanish on a single frustrated square while the absolute value of the bond correlations saturates at $1/2$. Hence, Eq. (7) remains valid and $1/3$ is to be replaced by $1/2$ in (6) and (11) whenever an edge of a square is considered. The estimates of N_n and N_n^{ij} depend on the particular model.

3. Analytical Behaviour of the Free Energy of Superfrustrated Models at $T = 0$

A singularity in the free energy is usually connected to the appearance of a genuine cooperative behaviour among infinitely many degrees of freedom. The singularity at zero temperature may present a remarkable exception [9]. Indeed, the free energy of a single Ising spin in an external field h ,

$$f_h = -k_B T \ln(2 \cosh(h / k_B T)) \quad (12)$$

also shows an essential singularity at $T = 0$. In fact, this type of singularity appears in the free energy of any Ising model with interactions $\{J_b\}$ (b is a single site, a pair of sites etc.), since the partition function can be written as

$$Z \sim \left(\prod_b \cosh(J_b / k_B T) \right) \sum_{\text{"closed graphs"}} \prod_b \tanh(J_b / k_B T) \quad (13)$$

These remarks indicate that the sign of an eventual cooperative behaviour at $T = 0$ is to be looked for in the second factor of (13). In our case, it is convenient to normalize the free energy according to the number of dominant plaquettes and to write

$$f = (\alpha f_t + (1 - \alpha) f_{sq}) + \psi \quad (14)$$

Here f_t and f_{sq} are the free energies of the isolated triangular and square plaquettes, respectively, and ψ represents the correction due to the interactions among the different plaquettes. For frustrated plaquettes f_t and f_{sq} are given by

$$f_{t,sq} = -k_B T \left[m \ln(\cosh J_{ij} / k_B T) + \ln \left(1 - \prod_{\substack{\langle ij \rangle \\ \text{plaquette}}} \tanh(|J_{ij}| / k_B T) \right) \right] \quad (15)$$

where $m=3$ in f_t and $m=4$ in f_{sq} ... As (13) and (15) show, ψ depends on T via $\tanh(J_{ij} / k_B T)$ or, after separating off the signs of the interactions, via $w \equiv \tanh(|J_{ij}| / k_B T)$. The singularity of f at $T = 0$ is there-

fore determined by the behaviour of f_t (and f_{sq}) around $T = 0$ and the behaviour of ψ around $w = 1$. As mentioned earlier, the former is not significant because it reflects the properties of a finite system. Hence, one concludes that any feature of the free energy which is particular to superfrustration, must appear in the $w = 1$ behaviour of the function ψ .

In Ref. [8], a comparative study of ψ for the KFF and SFF models was performed by localizing the zeros of the corresponding (reduced) partition functions on the complex w -plane. It was found that for the KFF model the $0 \leq w \leq 1$ segment lies in the interior of a domain free of zeroes while $w = 1$ is on the border of the domain of zeroes, for the SFF model. The proof uses nothing particular to the KFF model except the properties (i) - (iv). Hence, one can draw the following conclusion:

In an Ising model satisfying the conditions (i) - (iv), the part of the free energy which describes the interaction of different plaquettes is an analytic function of $w = \tanh(|J_{ij}| / k_B T)$ for $0 \leq w \leq 1$.

This property also shows that the name "superfrustration" is well justified: the frustration is so strong that it makes the infinite system to behave essentially like the union of independent small subsystems.

4. Sensitivity to the Boundary Condition in the Ground State and the Decay of the Correlation at $T = 0$

As [7] and the present Sect. 2 illustrate, a certain amount of mathematical work is needed to find the rate of decay of the pair correlation function in different frustration models. However, to convince ourselves that there must be a difference between the SFF and KFF models, it is sufficient to look at some general properties of the ground state configurations in the two cases.

It is well known that the correlations usually depend on the choice of the boundary condition which is maintained while the thermodynamic limiting process is performed. Instead of pair correlations, one may consider the magnetization at the origin, $\langle S_0 \rangle_{V,\delta}$, so that the spins are

fixed in the configuration \hat{S} outside the volume V . (\hat{S} may eventually be zero in some or all of the sites.)

If

$$\langle S_0 \rangle_{\hat{S}} = \lim_{V \rightarrow \infty} \langle S_0 \rangle_{V, \hat{S}}$$

depends on \hat{S} , this indicates that S_0 remains correlated with the boundary spins while the boundary disappears in the infinity. In such a case, the correlation length must be infinite which implies either a long range order or a power-law decay. If $\langle S_0 \rangle_{\hat{S}}$ does not depend on the boundary condition \hat{S} then one expects a finite correlation length, i.e., an exponential decay of the correlation.

Let us look at the TAF and SFF models. If a ground state configuration is singled out at random, it will almost surely be a configuration in which every spin can be freely flipped either by itself or together with a few other spins. If any of these non-isolated ground states is taken as the boundary condition \hat{S} , the infinite-volume correlations will not depend on the particular choice and will certainly give $\langle S_0 \rangle_{\hat{S}} = 0$. One may say that any of the non-isolated ground states (which form the overwhelming majority of the whole set of ground states), taken as boundary condition, determines one and the same phase of the system: a phase with a finite entropy per spin. There are, however, isolated ground states in the TAF and SFF models. Figure 1 shows a gauge-invariant representation of such a ground state in both cases: the frustrated bonds are crossed with a line segment. To flip the spins in a finite domain, the cost of energy is proportional to the length of the border of this domain minus the number of the frustrated bonds along the border. Starting from the ground states of Fig. 1, the energy cost of any local transformation is positive which means that the resulting configuration is not a ground state and therefore is not available at $T = 0$. Hence, taking an isolated ground state \hat{S} as the boundary condition, one obtains that

$$\langle \prod_{i \in B} S_i \rangle_{\hat{S}} = \prod_{i \in B} \hat{S}_i = \pm 1$$

for any set B of sites. This shows the existence of a zero temperature equilibrium state which is concentrated to the single configuration \hat{S} . It is found therefore that the infinite-volume correlations are sensitive to the boundary condition in the TAF and SFF models. According to our former speculation, this means the infinity of the correlation length: long range order if the boundary condition is an isolated ground state and power-law decay if it is non-isolated.

Unfortunately, I cannot give a rigorous proof to the claim that there is no isolated ground state in the KFF or generally, in the superfrustrated models. At least, my attempt to find such a configuration was unsuccessful. Figure 2 presents a ground state of the KFF model. It is to be noted that the model is overfrustrated which means that in any configuration there are plaquettes with more than one frustrated bond. Indeed, the ratio of the number of triangular and hexagonal plaquettes is 2:1, hence one cannot cover the lattice with triangle-hexagon pairs. If in a ground state every triangle has one frustrated bond and a portion γ of the hexagons has three of them then

$$2 = 3\gamma + (1 - \gamma)$$

which gives $\gamma = 1/2$. The ground state shown on Fig. 2 is of this kind. The absence of isolated ground states strongly suggests that the infinite-volume correlations do not depend on the boundary condition which is in agreement with the formerly found exponential law of decay.

In fact, as it was mentioned already in the Introduction, the stability of the set of the ground states against boundary perturbations is likely to be a sufficient and necessary condition for superfrustration. This condition can be formulated still in another way. We say that the set of the ground states is connected if for any two ground states S and S' there exists a sequence of ground states $S^1, S^2, \dots, S^n, \dots$ so that $S^1 \equiv S$, S^n is different from S^{n+1} only at a finite number of sites (for any n) and S^n tends to S' pointwise (i.e., for any site i there exists a number n_i such that $S_i^n = S'_i$ for any $n > n_i$). Now I summarize all the speculations of this section in the following conjecture:

A model is superfrustrated if and only if it has more than one ground state and the set of the ground states is connected.

If the Hamiltonian is invariant with respect to the global transformation $S \rightarrow -S$ then the above condition for the superfrustration is identical with that conjectured by Hoever et al.[10] for the absence of the breakdown of this symmetry. Hence, there is a strong indication that models with purely pair interactions are superfrustrated if and only if the global spin-flip symmetry is not violated in the $T=0$ equilibrium state.

However, our conjecture refers also to models the Hamiltonian of which has no internal symmetry. Clearly, in this latter case the condition (iv), given in the Introduction, is not satisfied. The conjecture can be used to get examples for models with such interactions, which are likely to be superfrustrated. Let me remind the reader that the general definition of the correlation length ξ comes from the asymptotic (large r) behaviour of the "truncated" correlation function :

$$\langle S_0 S_r \rangle - \langle S_0 \rangle \langle S_r \rangle \sim \exp (-r/\xi) \quad (16)$$

In the example treated in Sect.2, $\langle S_0 \rangle = \langle S_r \rangle = 0$ because of the purely pair interactions and the vacuum boundary condition; therefore, the finiteness of ξ follows from the exponential decay of $\langle S_0 S_r \rangle$. In the case of a frustration model with a Hamiltonian containing, for instance, an external field, the fact of the eventual superfrustration can be inferred from the exponential decay of the truncated correlation function at $T=0$.

Now, let us consider a two-sublattice antiferromagnet in a critical external field. The Hamiltonian of such a model can be written as

$$H = \sum_{\langle ij \rangle} S_i S_j - z \sum_i S_i \quad (17)$$

where the first sum runs over nearest neighbour pairs and z is the coordination number. The purely antiferromagnetic model is not frustrated on the same lattice but the competition between the external field and the antiferromagnetic interaction gives rise to frustration. Any configuration not containing negative nearest neighbour spins is a ground state. The two antiferromagnetic and the all-plus ferromagnetic ground states are connected to each other by local transformations in the sense defined above and it is rather obvious that the whole set of the ground states is also connected. Provided that our conjecture is correct, we obtain the following result:

Any two-sublattice Ising antiferromagnet in a critical external field is a model for the superfrustration.

There is, at least, one case in which a rigorous proof is possible: the antiferromagnetic chain in a critical field. Consider the model described by the Hamiltonian

$$H^{(1)} = \sum_i S_i S_{i+1} - 2 \sum_i S_i \quad (18a)$$

The effect of the external field can be simulated by a ferromagnetic coupling to two neighbouring chains in which the spins are frozen-in at the value +1. Let $\alpha(i)$ and $\beta(i)$ be the neighbours of the site i perpendicularly to the chain ; then

$$H^{(1)} = \sum_i S_i S_{i+1} - \sum_i (S_i S_{\alpha(i)} + S_i S_{\beta(i)}) \quad (18b)$$

provided that $S_{\alpha(i)} = S_{\beta(i)} = 1$ for all i . The magnetization in the model (18b) was studied in an earlier paper [11] dealing with the frustration models of Longa and Oleś [12]. It was found that for (18b) and, hence, for (18a) the magnetization at $T = 0$ in the infinite chain is

$$\langle S_i \rangle = 1/\sqrt{5} \quad (19)$$

for any site i . Using the results of [11], it is easy to calculate

$\langle S_0 S_r \rangle$. For a finite chain containing k spins above S_r and ℓ spins below S_0 , one obtains the following probabilities at $T = 0$:

$$\begin{aligned} \text{Prob}(S_0 = S_r = 1) &= n_k n_\ell n_{r-1} / n_{k+\ell+r+1} \\ \text{Prob}(S_0 = S_r = -1) &= n_{k-1} n_{\ell-1} n_{r-3} / n_{k+\ell+r+1} \\ \text{Prob}(S_0 = -S_r = 1) &= n_{k-1} n_\ell n_{r-2} / n_{k+\ell+r+1} \\ \text{Prob}(S_0 = -S_r = -1) &= n_k n_{\ell-1} n_{r-2} / n_{k+\ell+r+1} \end{aligned} \quad (20)$$

Here n_k is the number of ground states in a chain of k spins interacting via $H^{(1)}$. This number was calculated in [11]:

$$n_k = \frac{2\sqrt{5}+4}{5+\sqrt{5}} \left(\frac{1+\sqrt{5}}{2}\right)^k - \frac{2\sqrt{5}-4}{5-\sqrt{5}} \left(\frac{1-\sqrt{5}}{2}\right)^k \quad (21)$$

Taking the limits $k, \ell \rightarrow \infty$ in Eqs.(20) we find from (19), (20) and (21) that

$$\langle S_0 S_r \rangle - \langle S_0 \rangle \langle S_r \rangle = \frac{4}{5} \left(\frac{1-\sqrt{5}}{1+\sqrt{5}}\right)^r \quad (22)$$

According to (16) this means that the correlation length

$$\xi = 1 / \ln \frac{\sqrt{5}+1}{\sqrt{5}-1} \quad (23)$$

at $T = 0$, for the one dimensional antiferromagnetic chain in a critical external field.

5. Summary

In this work I discussed a family of Ising models in which the effect of frustration reaches its extremes. I found that the systems described by these so-called superfrustrated models show no cooperative behaviour at any $T \geq 0$: the correlation length remains finite and the free energy is essentially that of a finite system. Such models can be constructed in any dimension: the conditions (i) - (iv) have to be fulfilled. In particular, the example of the KFF model shows that not all the two dimensional fully frustrated models belong to the same universality class, in contrast to what was expected. This follows from the detailed calculations and is reflected also by the existence of

isolated ground states in the TAF and SFF models and their absence in the KFF model. A qualitative argument suggests that two-sublattice antiferromagnets in critical external fields are superfrustrated. This has been justified rigorously for the one dimensional model.

Acknowledgement

I am indebted to P. Erdős for his critical reading of the manuscript. I have much profited from several remarks of G. Toulouse and from a correspondence with P. Fazekas and W.F. Wolff.

References

1. G. Toulouse, Commun. Phys. 2 115 (1977)
2. G.H. Wannier, Phys. Rev. 79 357 (1950)
3. K. Kano and S. Naya, Prog. Theor. Phys. 10 158 (1953)
4. J. Villain, J. Phys. C: Solid St. Phys. 10 1717 (1977)
5. J. Stephenson, J. Math. Phys. 5 1009 (1964)
6. B.W. Southern, S. T. Chui and G. Forgacs, J. Phys. C: Solid St. Phys. 13 L827 (1980)
7. G. Forgacs, Phys. Rev. B 22 4473 (1980)
8. A. Sütö, Helv. Phys. Acta 54 (1981) in press
9. Another exception is the Griffiths singularity (R.B. Griffiths, Phys. Rev. Letters 23 17 (1969)) in random ferromagnets below the percolation threshold.
10. P. Hoever, W.F. Wolff and J. Zittartz, Z. Phys. B 41 43 (1981)
11. A. Sütö, J. Phys. A: Math. Gen. 14 (1981) in press
12. L. Longa and A.M. Oleś, J. Phys. A: Math. Gen. 13 1031 (1980)

Figure Captions

Figure 1 The frustrated bonds in an isolated ground state of the fully frustrated model
a) on the square lattice
b) on the triangular lattice.

Figure 2 The frustrated bonds in a ground state of the fully frustrated model on the Kagomé lattice.



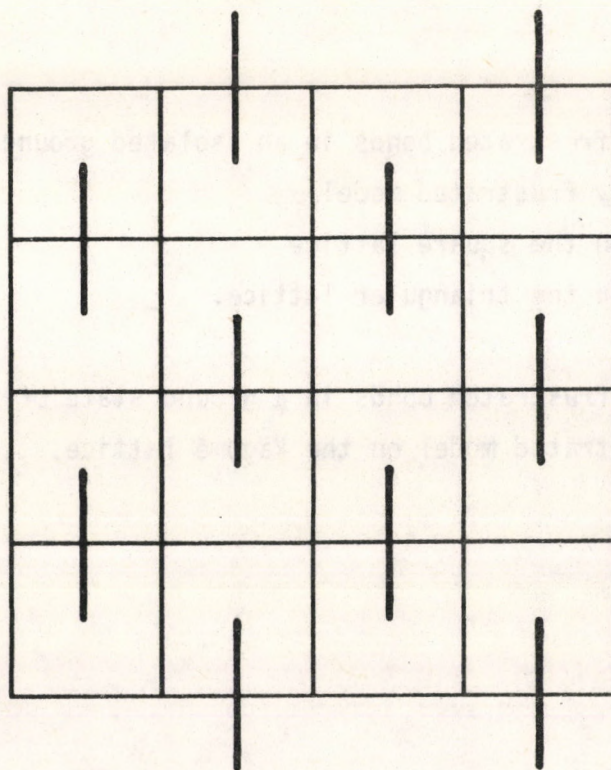


Fig. 1a.

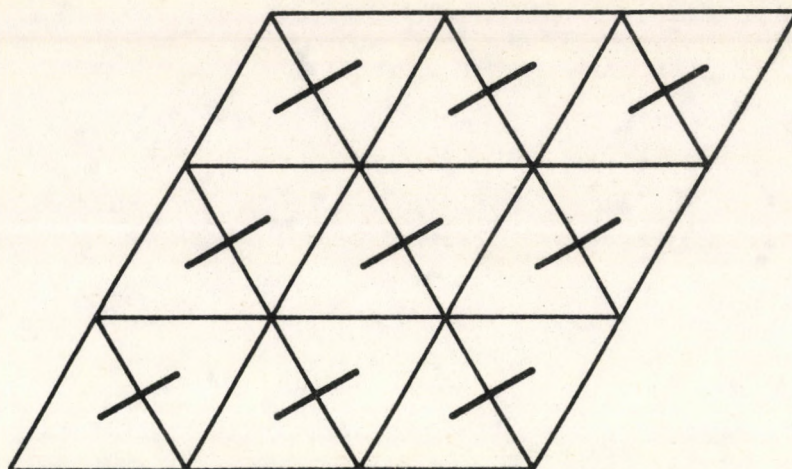


Fig. 1b.

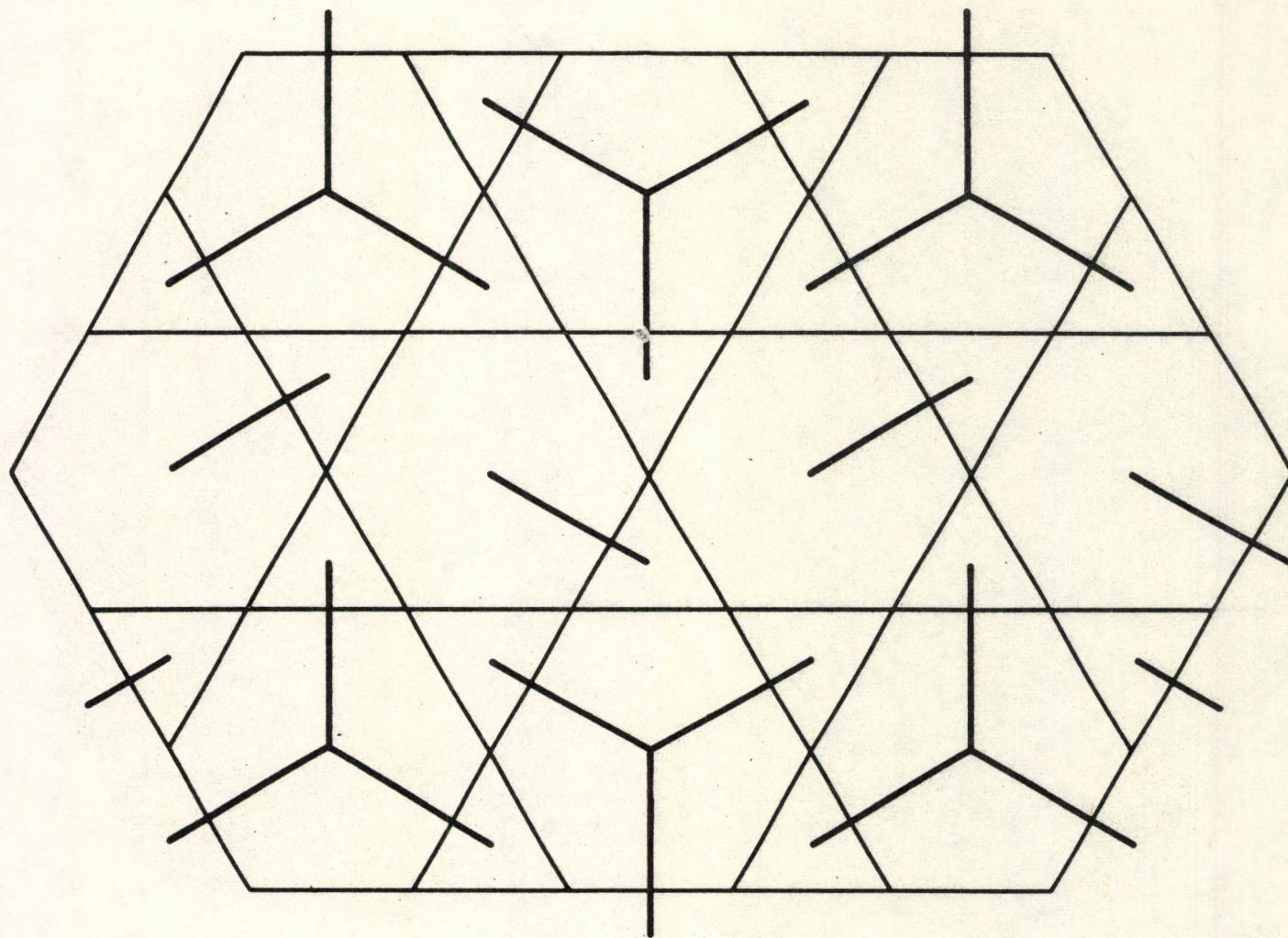


Fig. 2.





Kiadja a Központi Fizikai Kutató Intézet
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